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FILE COVERS 1907 - 24 Dec 2003  VOL 139 ISS 26
FILE LAST UPDATED: 23 Dec 2003  (20031223/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s  (paral?(w) mass (w)spectr?)
        321747 PARAL?
        788655 MASS
         71248 MASSES
        826335 MASS
                  (MASS OR MASSES)
       2285432 SPECTR?
L10         16 (PARAL?(W) MASS (W)SPECTR?)

=> d bib,abs 1-16

L10  ANSWER 1 OF 16  CAPLUS  COPYRIGHT 2003 ACS on STN
AN   2003:289440  CAPLUS
DN   139:193345
TI   A generic assay for phosphate-consuming or -releasing enzymes coupled
     on-line to liquid chromatography for lead finding in natural products
AU   Schenk, T.; Appels, N. M. G. M.; van Elswijk, D. A.; Irth, H.; Tjaden, U.
     R.; van der Greef, J.
CS   Kiadis B.V., Leiden, 2333 CA, Neth.
SO   Analytical Biochemistry (2003), 316(1), 118-126
     CODEN: ANBCA2; ISSN: 0003-2697
PB   Elsevier Science
DT   Journal
LA   English
AB   A generic continuous-flow assay for phosphate-consuming or -releasing
     enzymes coupled online to liq. chromatog. (LC) has been developed.
     Operating the LC-biochem. assay in combination with mass spectrometry
     allows the fast detection and identification of inhibitors of these
     enzymes in complex mixts.  The assay is based on the detection of
     phosphate, released by the online continuous-flow enzymic reaction, using
     a fluorescent probe.  The probe consists of fluorophore-labeled
     phosphate-binding protein, which shows a strong fluorescence enhancement
     upon binding to inorg. phosphate.  To detect very small changes of the
     phosphate concn. in a postcolumn enzymic reaction medium, the enzymic
     removal of phosphate impurities from solvents, reagents, and samples was
     optimized for application in continuous flow.  The potential of the
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phosphate probe is demonstrated by monitoring the enzymic activity, i.e., the phosphate release, from alk. phosphatase. The selectivity of the phosphate readout, necessary to distinguish between phosphate contg. substrate or product and free inorg. phosphate released after enzymic conversion, is shown. The applicability of LC coupled to the enzymic assay using the phosphate readout was demonstrated by detection of tetramisole in a plant ext. as inhibitor of alk. phosphatase. **Parallel mass spectrometry** allowed the simultaneous confirmation of the identity of the inhibitor.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:949675 CAPLUS
DN 139:134016
TI TEM Imaging of Mass-selected Polymer Molecules
AU Nasibulin, Albert G.; Kauppinen, Esko I.; Thomson, Bruce A.; Fernandez de la Mora, J.
CS Aerosol Technology Group, VTT Processes, FIN-02044, Finland
SO Journal of Nanoparticle Research (2002), 4(5), 449-453
CODEN: JNARFA; ISSN: 1388-0764
PB Kluwer Academic Publishers
DT Journal
LA English
AB Polyethylene glycol (PEG) mols. with masses below 1300 amu are electrosprayed (ES) from soln., mobility-selected at high resoln. in a differential mobility analyzer (DMA), collected on a grid and imaged by transmission electron microscopy (ES-DMA-TEM). The DMA resolves individual n-mers, and selects only one out of the many present in the original sample. Ion identity is established from **parallel mass spectra** (ES-MS). The images reveal spherical particles 1.46 nm in diam., in good agreement with the known ion mass and bulk d. The DMA-selection technique opens new paths for the study of very small particles.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:688793 CAPLUS
DN 137:358560
TI Thermal Stability of Self-Assembled Monolayers: Influence of Lateral Hydrogen Bonding
AU Valiokas, Ramunas; Oestblom, Mattias; Svedhem, Sofia; Svensson, Stefan C. T.; Liedberg, Bo
CS Division of Applied Physics, Division of Chemistry, Department of Physics and Measurement Technology, Linkoepings Universitet, Linkoeping, S-581 83, Swed.
SO Journal of Physical Chemistry B (2002), 106(40), 10401-10409
CODEN: JPCBFK; ISSN: 1520-6106
PB American Chemical Society
DT Journal
LA English
AB Temp.-programmed desorption (TPD) of self-assembled monolayers (SAMs) on Au is studied by using in **parallel mass spectrometry** (MS) and IR reflection-absorption spectroscopy (IRAS). Monolayers formed by HS(CH2)n-OH (n = 18, 22) and HS(CH2)15-CONH-(CH2CH2O)-H (EG1) are compared to reveal the influence of specifically introduced hydrogen-bonding groups on their thermal stability. The overall desorption process of the above mols. occurs in 2 main steps; a disordering of the alkyl chains followed by a complex series of decompn./desorption reactions. The final step of the process involves desorption of S from different chemisorption states. The amide-group-contg. SAM, which is stabilized by lateral hydrogen bonds, displays a substantial delay of the alkyl chain disordering by .apprx.50

K, as compared to the linear chain alcs. HS(CH2)n-OH. also, the decompn. of the alkyls and the onset of S desorption occur at a temp. that is higher by .apprx.25 K as compared to the HS(CH2)18-OH SAM. The desorption process is also studied for 2 oligo(ethylene glycol)-terminated SAMs, HS(CH2)15-X-(CH2CH2O)4-H (EG4-SAMs), where X is -CONH- and -COO- linking groups. In addn. to the mol. chain disordering, the decompn./desorption process of the EG4-SAMs occurs in 2 steps. The 1st is assocd. with the loss of the oligomer portion and the 2nd with the desorption of the alkylthiolate part of the mol. Study points out that lateral hydrogen bonding, introduced via amide groups, is a convenient way to improve the thermal stability of alkanthiolate SAMs.

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:59880 CAPLUS
DN 136:262794
TI Neutral products from gas phase rearrangements of simple carbocations
AU Morton, Thomas Hellman
CS Department of Chemistry, University of California, Riverside, CA, 92521-0403, USA
SO Advances in Gas Phase Ion Chemistry (2001), 4, 213-256
CODEN: AGPCER; ISSN: 1071-9687
PB JAI Press Inc.
DT Journal; General Review
LA English
AB A review; analyzing the neutral products from ionic reactions in the gas phase provides information that cannot be gained by mass spectrometric methods alone. Neutrals have been recovered using three general techniques for generating ions in sufficient quantities: nuclear decay of multiply tritiated precursors, .gamma.-radiolysis studies, and electron bombardment flow (EBFlow) expts. Analyses of the uncharged reaction products of ion-mol. reactions are most effectively interpreted in conjunction with **parallel mass spectrometric** investigations. Taken together, these combined studies demonstrate the propensity of gaseous cations to undergo similar sorts of isomerizations as have been reported in condensed media. The absence of solvent and counterions makes it possible to produce ions in the gas phase that cannot be formed in soln. Despite the difference in reaction medium, the same two general categories of rearrangement-ring closure/ring opening and atom/group transfer-account for the variety of ion structures that give rise to the obsd. neutral products.

RE.CNT 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:106149 CAPLUS
DN 133:101503
TI A multiple electrospray interface for **parallel mass spectrometric** analyses of compound libraries
AU Wang, T.; Zeng, L.; Cohen, J.; Kassel, Daniel B.
CS CombiChem, Inc., San Diego, CA, USA
SO Combinatorial Chemistry and High Throughput Screening (1999), 2(6), 327-334
CODEN: CCHSFU; ISSN: 1386-2073
PB Bentham Science Publishers
DT Journal
LA English
AB A parallel spray interface for mass spectrometry is described. This new electrospray interface enables effluent flow streams from an array of HPLC columns to be sampled independently and sequentially on a chromatog. time-scale. Unlike our previously reported parallel LC-MS interface, which incorporated a dual-sheath spray interface accommodating up to four flow streams that are sampled simultaneously, this new interface permits

up to four columns to be sampled sequentially by means of a stepping motor and rotating plate assembly. Effluent flow streams from an array of four HPLC columns are connected to a parallel arrangement of electrospray needles co-axial to the mass spectrometer entrance aperture. Within the needle assembly, the individual spray tips are oriented in a circular array, where each needle is situated 90 degrees relative to one another for four-column operation. An eight-column system is described with needles spaced at 45 degree intervals. In between the needle assembly and the mass spectrometer entrance aperture is a Teflon disk with a through-hole that is mounted to a stepping motor assembly. By precisely controlling the stepping of the motor assembly, it is possible to "sample" each of the spray positions multiple times per s. By operating the quadrupole mass spectrometer in the single ion monitoring (SIM) mode, it was possible to acquire data at each of the spray positions during the course of the elution of compds. from the HPLC column array while maintaining both good sensitivity and peak shape. Preliminary results suggest this technique will be useful for high throughput combinatorial library anal. and profiling.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:148610 CAPLUS
DN 128:267854
TI Dual **parallel mass spectrometers** for analysis of sphingolipid, glycerophospholipid and plasmalogen molecular species
AU Byrdwell, Wm. Craig
CS FQS, NCAUR, ARS, USDA, Peoria, IL, 61604, USA
SO Rapid Communications in Mass Spectrometry (1998), 12(5), 256-272
CODEN: RCMSEF; ISSN: 0951-4198
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB Anal. of phospholipids was performed using a liq. chromatog. sepn. with two mass spectrometers in parallel providing electrospray ionization (ESI) and atm. pressure chem. ionization (APCI) data simultaneously from a triple quadrupole instrument and a single quadrupole instrument, resp. The output from UV-Vis and evaporative light scattering detectors were also acquired by the two mass spectrometers, resp., for four detectors overall. This arrangement was used to identify and calc. area percents for mol. species of dihydrosphingomyelin (DHS) and sphingomyelin (SPM) in com. available bovine brain SPM, in human plasma ext. and in porcine lens ext. Mol. species of phosphatidylethanolamine and its plasmalogen, and phosphatidylcholine and its plasmalogen were identified and semi-quant. anal. performed. Com. available bovine brain SPM was found to contain 11.5% DHS and 88.5% SPM. The only DHS mol. species identified in human plasma was 16:0-DHS, at or below 1% of the sphingolipid content. Porcine lens membranes were found to contain 14.4% DHS and 85.6% SPM. Other findings reported here include: (1) phospholipids were found to undergo dimerization in the electrospray source, giving masses representing combinations of species present. (2) Triacylglycerols gave usable mass spectra under electrospray ionization conditions, as well as under APCI-MS conditions. (3) Triacylglycerols gave ammonium adducts as base peaks in their APCI mass spectra, which reduced fragmentation and increased the proportions of mol. ions. (4) Mass spectra were obtained for phospholipids which underwent both protonation and sodium adduct formation in different chromatog. runs. This paper was prepd. under the auspices of the US Government and it is therefore not subject to copyright in the US.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:45137 CAPLUS

DN 128:75016
TI Methanol Oxidation on Rhodium As Probed by Surface-Enhanced Raman and Mass Spectroscopies: Adsorbate Stability, Reactivity, and Catalytic Relevance
AU Williams, Christopher T.; Takoudis, Christos G.; Weaver, Michael J.
CS School of Chemical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN, 47907, USA
SO Journal of Physical Chemistry B (1998), 102(2), 406-416
CODEN: JPCBFK; ISSN: 1089-5647
PB American Chemical Society
DT Journal
LA English
AB The relationship between surface speciation and catalytic activity/selectivity during methanol oxidn. on polycryst. rhodium under ambient-pressure flow-reactor conditions was studied from 25 to 500 .degree.C by means of surface-enhanced Raman spectroscopy (SERS) along with **parallel mass spectrometric** (MS) measurements. By utilizing SERS-active Rh films formed by electrodeposition onto gold, the former technique provides in situ surface vibrational spectra with unique sensitivity under these demanding conditions, enabling adsorbed species to be probed in real time (.apprxeq.1 s) for comparison with the overall kinetics as evaluated by MS. Exposure of Rh to O2-free methanol yielded no detectable vibrational bands between 25 and 500.degree., although methanol decompn. to form CO and H2 was evident from MS. The presence of even subunity molar ratios of oxygen, however, yielded rich SER spectra, highlighted by bands indicative of CO(ads) (.nu.Rh-CO = 465 cm-1, .nu.Rh-CO = 2000 cm-1). The catalytic selectivity toward CO2 (vs. CO) gaseous product formation decreased markedly around the desorption temp. of CO(ads) .apprxeq. 350.degree. under these conditions. This is consistent with the facilitation of CO2 prodn. by the presence of CO(ads). Complete selectivity toward exhaustive methanol oxidn. (i.e., CO2, H2O formation) was obsd. in oxygen-rich methanol mixts., adsorbed CO now being absent at all temps. The CO2 prodn. occurs partly via methanolic C-O cleavage as deduced by 1802 substitution. The presence of rhodium oxide (Rh2O3) was diagnosed with such reactant mixts. above ca. 300 .degree.C from the characteristic 500-580 cm-1 .nu.Rh-O bands. The kinetics of formation and removal of the oxide were probed by gas flow switching coupled with transient SERS measurements. The oxide formation rates following O2 exposure are slowed markedly (>100-fold) by the presence of even a small (5%) methanol mole fraction. Switching to pure methanol results in very rapid oxide redn., so that, for example, removal is complete within ca. 1s at 350.degree. with 100 Torr of CH3OH. Examn. of the transient oxide removal kinetics as a function of temp. and methanol pressure revealed a transition from strongly activated to essentially T-independent behavior at lower pressures and/or higher temps. This is indicative of a change from rate-detg. removal of oxygen from the oxide lattice to a subsequent step involving formation of and/or reaction with an adsorbed methanol scavenger. While such reactivity earmarks the oxide as a potential reaction intermediate, the overall catalytic turnover rates for methanol oxidn. are nonetheless faster than can be accommodated on this basis.
RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:410724 CAPLUS
DN 127:155996
TI Probing Combinatorial Library Diversity by Mass Spectrometry
AU Demirev, Plamen A.; Zubarev, Roman A.
CS Division of Ion Physics The Aangstroem Laboratory, Uppsala University, Uppsala, S-751 21, Swed.
SO Analytical Chemistry (1997), 69(15), 2893-2900
CODEN: ANCHAM; ISSN: 0003-2700
PB American Chemical Society
DT Journal

LA English
AB The feasibility of a massively **parallel mass spectrometric** method for probing combinatorial library diversity is addressed theor. for the example of computer-generated mass distributions of combinatorially synthesized peptide libraries contg. between two and seven amino acids. The authors study the behavior of several global (integral) parameters of such mass distributions-mass centroid, dispersion, skewness, and kurtosis. The centroid and dispersion carry information that may characterize the completeness of the synthetic effort. Local mass distribution parameters, e.g., mass d. (no. of peptides per mass interval), are also examd. The practical implementation and eventual limitations of such an approach are discussed as well.

L10 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:667782 CAPLUS
DN 125:320017
TI Detection of the picolinic acid biomarker in Bacillus spores using a potentially field-portable pyrolysis-gas chromatography-ion mobility spectrometry system
AU Snyder, A. Peter; Thornton, Sidney N.; Dworzanski, Jacek P.; Meuzelaar, Henk L. C.
CS Dev. Eng. Cent., U.S. Army Edgewood Res., Aberdeen Proving Ground, MD, 21010-5423, USA
SO Field Analytical Chemistry and Technology (1996), 1(1), 49-59
CODEN: FACTFR; ISSN: 1086-900X
PB Wiley
DT Journal
LA English
AB The absence of a field-portable device to provide real-time detection of Gram-pos. bacterial spores has prompted the interfacing of a pyrolysis (Py) module to an existing, hand-held gas-chromatog.-ion-mobility spectrometry (GC/IMS) device. In this configuration, spore detection is achieved by the observation of picolinic acid (PA), which is the most characteristic pyrolysis decompn. product of the parent dipicolinic (2,6-pyridinedicarboxylic) acid (DPA). Pos. identification of PA was demonstrated using a lab.-based GC instrument with dual, **parallel mass spectrometry** (MS) and IMS detectors. Spores and vegetative microorganisms of the genus Bacillus were characterized by the presence and absence of DPA, resp., and the picolinic acid marker was identified from the GC/IMS and GC/MS profiles. A field-portable prototype Py-GC/IMS system is described and appears to provide similar bioanal. information with respect to the lab.-based system. Preliminary results of this study indicate that the degree of compd. sepn. afforded by a short GC capillary column guards against common environmental interferences including urban particulate matter and biol. particles such as fungal spores and pollen.

L10 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1987:429781 CAPLUS
DN 107:29781
TI Determination of the nuclear reactor burning process balance by gamma spectrometry of fission products. Part V - Determination of the isotopic composition of irradiated uranium
AU Bulovic, V.; Maksimovic, Z.; Krtil, J.; Sus, F.; Klosova, E.
CS Boris Kidric Inst. Nucl. Sci., Vinca, Yugoslavia
SO Jaderna Energie (1987), 33(1), 8-11
CODEN: JADEAQ; ISSN: 0448-116X
DT Journal
LA English
AB The possibility of detg. the isotopic compn. of irradiated U fuel of a heavy water reactor on the basis of .gamma.-spectrometry of fission products was exptl. tested. The testing was performed upon spent fuel from unenriched U. For detg. the fission products (106Ru, 134Cs and 137Cs) a spectrometer with a Ge(Li) detector was used. The accuracy of

the results obtained for the compn. of U was tested through its **parallel mass-spectrometric** analyses.

L10 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1987:112632 CAPLUS
DN 106:112632
TI The thermal decomposition of strontium fluorophosphate hydrate (SrPO3F.cntdot.H2O)
AU Menz, D. H.; Heide, K.; Kunert, C.; Mensing, C.; Kolditz, L.
CS Zentralinst. Anorg. Chem., Dtsch. Akad. Wiss., Berlin, DDR-1199, Ger. Dem. Rep.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1986), 540-541, 191-7
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
AB The thermal decompn. of SrPO3F.H2O was studied by complex thermal anal. The thermogravimetric study was completed by simultaneous and **parallel mass spectrometric** anal. of the gas phase. During the 1st state of thermal decompn. .apprx.0.8 mol water is lost. Then a partial hydrolysis takes place and HF is formed. The formation of POF3 is a multistage mechanism without effect of H2O at >500.degree.. The partial reactions leading to .alpha.-Sr2P2O7 and SrF2 >600.degree. and to .alpha.-Sr2P2O7 and Sr5(PO4)3F >750.degree. were formulated and the exptl. and calcd. mass loss were compared.

L10 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1985:196916 CAPLUS
DN 102:196916
TI Thermal decomposition of calcium phosphorofluoridate dihydrate (CaPO3F.2H2O)
AU Heide, K.; Menz, D. H.; Schmidt, C.; Kolditz, L.
CS Sekt. Chem., Friedrich-Schiller-Univ., Jena, DDR-6900, Ger. Dem. Rep.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 520, 32-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
AB The thermal decompn. of CaPO3F.2H2O was studied by thermogravimetry under inert conditions. A **parallel mass spectrometric** anal. of gases produced was made. With the use of an effusion cell a quasiequil. evapn. in the vicinity of the ion source of the spectrometer was achieved. The results are comparable with the thermogravimetric anal. under normal pressure. During 1st stage of thermal decompn. 1 mol H2O was lost. The further course is detd. by release of HF and POF3. The several steps of decompn. leading to .alpha.-Ca2P2O7 at >360.degree. are discussed.

L10 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1985:178482 CAPLUS
DN 102:178482
TI Method and apparatus for **parallel mass spectrometry**
PA Chang, Chuang, USA
SO Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59176663	A2	19841006	JP 1984-41208	19840303
	US 4507555	A	19850326	US 1983-472161	19830304
PRAI	US 1983-472161		19830304		

AB The design is claimed of a **parallel mass spectrometric** app. joined in tandem with a gas chromatograph.

L10 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1985:159764 CAPLUS
DN 102:159764
TI **Parallel mass spectrometry** for high performance GC and LC detection
AU Chang, C.
CS Wright State Univ., Dayton, OH, USA
SO American Laboratory (Shelton, CT, United States) (1985), 17(3), 59-64, 66
CODEN: ALBYBL; ISSN: 0044-7749
DT Journal; General Review
LA English
AB A review with 15 refs. Problem areas in using conventional scanning mass spectrometers for high-performance gas chromatog. (GC) and liq. chromatog. (LC) detection are discussed. The potential use of **parallel mass spectrometers** to avoid these problems is also discussed.

L10 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1976:600351 CAPLUS
DN 85:200351
TI Valence level photoelectron spectra of some heavy group 4-6 diatomic molecules
AU Wu, M.; Fehlner, T. P.
CS Dep. Chem., Univ. Notre Dame, Notre Dame, IN, USA
SO Journal of the American Chemical Society (1976), 98(24), 7578-85
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB The He I photoelectron spectra of GeS, GeSe, SnS, SnTe, and PbTe in the gas phase were obtained by the photoionization of the vapors above appropriate solids at 700-1000.degree.K. Spectra are assigned by using obsd. relative band areas, vibrational fine structure, and spin-orbit splitting along with electron impact ionization potentials and **parallel mass spectrometric** studies. There is significant mixing of the .SIGMA.1/2 and .PI.1/2 states in the heavier species. Distinct differences between the .PI. states of light and heavy diatomics are obsd. Similarities and differences between the valence regions of group 4-6 diatomics and diatomics of group 5-5 and group 3-7 are also reported.

L10 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1959:15979 CAPLUS
DN 53:15979
OREF 53:2923h-i,2924a
TI Anomalous behavior of gem-diethers in the mass spectrometer
AU LeBlanc, R. Bruce
CS Dow Chem. Co., Freeport, TX
SO Anal. Chem. (1958), 30, 1797-9
CODEN: ANCHAM; ISSN: 0003-2700
DT Journal
LA Unavailable
AB gem-Diether (compds. with 2 alkoxy groups on the same C atom) were measured in the mass spectrometer. They give different spectra, depending on whether the filament is bare W or carbonized W. The carbonized filament gives the normal spectrum. The bare filament causes a partial decompn. into a vinyl ether and alc. For example, MeCH(OEt)2 on decompn. yields EtOH and CH2:CHOEt. For reliable analysis of the compds. a carbonized filament is recommended.

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     (FILE 'WPIDS' ENTERED AT 16:18:38 ON 24 DEC 2003)

     FILE 'USPATFULL' ENTERED AT 16:21:50 ON 24 DEC 2003
L4             1 S   (PARALLEL(W) MASS (W)SPECTROMETRY)/TI,AB.CLM
L5             2 S   (PARALLEL(W) MASS (W)SPECTROMETRY)/TI,AB,CLM
L6             3 S   (PARALLEL(W) MASS (W)SPECTR?)/CLM,AB,TI
L7             3 S   (PARAL?(W) MASS (W)SPECTR?)/CLM,AB,TI
L8             9 S   (PARAL?(W) MASS (W)SPECTR?)
L9             8 S L8 AND PROTEIN

=> d bib,kwic 1-8

L9   ANSWER 1 OF 8  USPATFULL on STN
AN     2003:173349  USPATFULL
TI     System and method for high throughput screening of droplets
IN     Hess, Robert, Arlington, MA, UNITED STATES
       Brenan, Colin, Marblehead, MA, UNITED STATES
       Linton, John, Lincoln, MA, UNITED STATES
       Ozbal, Can, Cambridge, MA, UNITED STATES
       Green, Donald, Watertown, MA, UNITED STATES
       Hunter, Ian, Lincoln, MA, UNITED STATES
PI     US 2003119193       A1   20030626
AI     US 2002-267912      A1   20021008 (10)
RLI    Continuation-in-part of Ser. No. US 2001-842361, filed on 25 Apr 2001,
       PENDING
DT     Utility
FS     APPLICATION
LREP   BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618
CLMN   Number of Claims: 90
ECL    Exemplary Claim: 1
DRWN   14 Drawing Page(s)
LN.CNT 2283
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
SUMM   . . . speeds at which large numbers of samples can be analyzed.
       Unlike optical-based assays in which samples can be analyzed in
       parallel, mass spectrometry is a serial
       process in which sample must be analyzed one-at-a-time. Typically, a
       slow desalting step or purification step is. . .
SUMM   . . . seconds. In various embodiments, the rate is substantially one
       assay per second. The reaction may also be buffered only by
       proteins intrinsic to the assay such as the enzyme in an enzyme
       inhibition assay.
DETD   [0121] .alpha.-Chymotrypsin is a protease that cleaves proteins
       and peptides at aromatic amino acids such as phenylalanine, tyrosine,
       and tryptophan. The example assay attempts to discover inhibitors of.
       .

L9   ANSWER 2 OF 8  USPATFULL on STN
AN     2002:268969  USPATFULL
TI     Mass spectrometer apparatus for analyzing multiple fluid samples
       concurrently
IN     Moini, Mehdi, Austin, TX, United States
       Jiang, Longfei, Austin, TX, United States
PA     Board of Regents, The University of Texas System, Austin, TX, United
       States (U.S. corporation)
PI     US 6465776          B1   20021015
AI     US 2000-586588           20000602 (9)
DT     Utility
FS     GRANTED
EXNAM  Primary Examiner: Lee, John R.; Assistant Examiner: Vanore, David A.
LREP   Fulbright & Jaworski, LLP
CLMN   Number of Claims: 24
ECL    Exemplary Claim: 1
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DRWN 2 Drawing Figure(s); 2 Drawing Page(s)
LN.CNT 713
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
SUMM . . . of dual ESI sprayers have been tried with a Y-shaped orifice defined within the nozzle in order to investigate electrosprayed **proteins** using ion-ion or ion-molecule reactions. In particular the accurate measurement of masses of organic compounds has been another use of. . .
SUMM . . . Corporation on a "Hot Gas Sampling"; and U.S. Pat. No. 4,507,555 patented Mar. 26, 1985 to C. Chang on a **"Parallel Mass Spectrometer"**; and U.S. Pat. No. 4,562,351 patented Dec. 31, 1985 to P. Atherton et al and assigned to VG Instruments Group. . .

L9 ANSWER 3 OF 8 USPATFULL on STN
AN 2002:191521 USPATFULL
TI Massive parallel method for decoding DNA and RNA
IN Ju, Jingyue, Englewood Cliffs, NJ, UNITED STATES
Li, Zengmin, New York, NY, UNITED STATES
Edwards, John Robert, New York, NY, UNITED STATES
Itagaki, Yasuhiro, New York, NY, UNITED STATES
PI US 2002102586 A1 20020801
US 6664079 B2 20031216
AI US 2001-972364 A1 20011005 (9)
RLI Continuation-in-part of Ser. No. US 2000-684670, filed on 6 Oct 2000, PENDING
PRAI US 2001-300894P 20010626 (60)
DT Utility
FS APPLICATION
LREP John P. White, Cooper & Dunham LLP, 1185 Avenue of the Americas, New York, NY, 10036
CLMN Number of Claims: 60
ECL Exemplary Claim: 1
DRWN 28 Drawing Page(s)
LN.CNT 1869
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
SUMM [0034] The invention provides a **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .
DRWD [0057] FIG. 24: **Parallel mass spectrometry** system for DNA sequencing. Example shows three mass spectrometers in parallel. Samples are injected into the ion source where they. . .
DETD . . . In one embodiment, the mass tag is a 2-nitro-.alpha.-methyl-3,4-dimethoxybenzyl group. In one embodiment, the mass tag is detected using a **parallel mass spectrometry** system which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .
DETD [0133] The invention provides a **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .
DETD . . . areas of biomedical research. Though these ionization methods are suitable for the analysis of bioorganic molecules, such as peptides and **proteins**, improvements in both detection and sample preparation are required for implementation of mass spectrometry for DNA sequencing applications. Since the. . .
DETD [0151] The photocleavable 2-nitrobenzyl moiety has been used to link biotin to DNA and **protein** for efficient removal by UV light (.about.350 nm) (Olejnik et al. 1995, 1999). In the approach disclosed herein the 2-nitrobenzyl. . .
DETD . . . not capped. As discussed above, the photo cleavable 2-nitro benzyl moiety has been used to link biotin to DNA and **protein** for efficient removal by UV light (.about.350 nm) irradiation (Olejnik

et al. 1995, 1999). Four different 2-nitro benzyl groups with. . .

DETD [0172] To make mass spectrometry competitive with a 96 capillary array method for analyzing DNA, a **parallel mass spectrometer** approach is needed. Such a complete system has not been reported mainly due to the fact that most of the. . .

DETD [0173] A complete **parallel mass spectrometry** system includes multiple APCI sources interfaced with multiple analyzers, coupled with appropriate electronics and power supply configuration. A mass spectrometry. . . figures show a system with three mass spectrometers in parallel. Higher throughput is obtained using a greater number of in **parallel mass spectrometers**.

CLM What is claimed is:
26. The method of claim 17, wherein the mass tag is detected using a **parallel mass spectrometry** system which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .
54. A **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. .

L9 ANSWER 4 OF 8 USPATFULL on STN
AN 2002:133513 USPATFULL
TI Proteomic analysis by **parallel mass spectrometry**
IN LaPine, James R., Uxbridge, MA, UNITED STATES
Jardine, Ian, Los Gatos, CA, UNITED STATES
Story, Mike S., Los Gatos, CA, UNITED STATES
PI US 2002068366 A1 20020606
AI US 2001-835273 A1 20010413 (9)
PRAI US 2000-196889P 20000413 (60)
DT Utility
FS APPLICATION
LREP John J. Gagel, Fish & Richardson P.C., 225 Franklin Street, Boston, MA, 02110-2804
CLMN Number of Claims: 28
ECL Exemplary Claim: 1
DRWN 7 Drawing Page(s)
LN.CNT 1181
TI Proteomic analysis by **parallel mass spectrometry**

SUMM [0002] This invention relates to proteomic analysis by **parallel mass spectrometry**.

SUMM [0003] Within a typical cell there are several thousand **proteins**, its "proteome," which carry out the metabolic work of the cell. These **proteins** are in constant interplay with one another, and with every other sort of biomolecule found within a cell. The **proteins** physically interact, or bind, to each other and to common secondary molecules. The result of such interactions is a fine control and balancing of metabolic functions. For example, one **protein** may increase or decrease the function of another **protein** by binding to it and altering its structure by the addition or removal of a modifying group such as a phosphate. Another mode of action is for one **protein** to produce more or less of a secondary substance that interacts allosterically with a second **protein** (or multiple second **proteins**) to modulate its function. Analysis of the abundance of **proteins** can therefore be useful in elucidating the molecular basis of differences brought about by diseases or by therapeutic treatments

SUMM [0004] A number of techniques have been suggested for analyzing cellular **proteins**, including, for example, two-dimensional electrophoresis followed by mass spectrometry. In the case of two-dimensional electrophoresis, a **protein** sample is placed in

array to a common computing device, said mass spectral data being indicative of the identity and the abundance of **protein** in said multiple sample, and correlating said mass spectral data as a function of time.

2. The method of claim 1 comprising displaying said correlated data as a function of **protein** identity, **protein** abundance, and time.

4. The method of claim 1 comprising identifying **proteins** based on changes in abundance as a function of time.

6. The method of claim 4 comprising analyzing 500 **proteins** or more.

7. The method of claim 6 comprising analyzing 5000 **proteins** or more.

22. A method for analysis of **proteins** in a biological system comprising: providing a biological system containing **proteins** ; exposing the biological system to a stimulus; after exposing the biological system to the stimulus, sampling the biological system at multiple time intervals to obtain multiple samples; treating the multiple samples by a separation technique to provide multiple **protein** samples suitable for analysis by mass spectrometry; providing a parallel array of mass spectrometer systems capable of simultaneous analysis of as many **protein** samples as there are spectrometer systems in said array; analyzing the multiple **protein** samples in said parallel array of mass spectrometry systems to generate mass spectral data indicative of the identity and the abundance of **proteins** in said multiple **protein** samples; and in a common electronic computing device communicating with each of said mass spectrometry systems, correlating said mass spectral. . .

27. The system of claim 26 wherein the analysis includes analysis of about 500 **proteins** or more.

L9 ANSWER 5 OF 8 USPATFULL on STN
AN 1999:18911 USPATFULL
TI Methods and apparatus for sequencing polymers with a statistical certainty using mass spectrometry
IN Patterson, Dale H., Nashua, NH, United States
PA PerSeptive Biosystems, Inc., Framingham, MA, United States (U.S. corporation)
PI US 5869240 19990209
AI US 1995-447175 19950519 (8)
DT Utility
FS Granted
EXNAM Primary Examiner: Jones, W. Gary; Assistant Examiner: Rees, Dianne
LREP Testa, Hurwitz & Thibeault, LLP
CLMN Number of Claims: 47
ECL Exemplary Claim: 1
DRWN 16 Drawing Figure(s); 16 Drawing Page(s)
LN.CNT 1668
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
SUMM . . . complete primary structure identification. To date, Edman sequencing and adaptations thereof are the most widely used tools for sequencing certain **protein** and peptides residue by residue, while the enzymatic synthesis method is preferred for sequencing oligonucleotides.
SUMM In the case of **protein** and peptide sequencing, C-terminal sequencing via chemical methods has proven particularly difficult while being only marginally effective, at best. (See, e.g., Spiess, J. (1986)

Methods of **Protein** Characterization: A Practical Handbook (Shively, J. E. ed., Humana Press, N.J.) pp. 363-377; Tsugita et al. (1994) J. **Protein** Chemistry 13:476-479). Consequently, the C-terminus remains a region often not analyzed because of lack of a dependable method.

SUMM . . . offer a simple approach by which amino acids can be sequentially cleaved residue by residue from the C-terminus of a **protein** or a peptide. Carboxypeptidase Y (CPY), in particular, is an attractive enzyme because it non-specifically cleaves all residues from the. . .

SUMM . . . by residue. Not only is this approach labor-intensive, but it is complicated by amino acid contaminants in the enzyme and **protein**/peptide solutions, as well as by enzyme autolysis. A further hindrance to any sequencing effort of this type is the absolute. . .

SUMM . . . analysis such as field desorption (Hong et al. (1983) Biomed. Mass Spectrom. 10:450-457), electrospray (Smith et al. (1993) 4 Techniques **Protein** Chem. 463-470), and thermospray (Stachowiak et al. (1988) J. Am. Chem. Soc. 110:1758-1765), it is possible to perform direct mass. . .

SUMM . . . digestion of peptides has been combined with other mass spectrometry methods such as plasma desorption (Wang et al. (1992) Techniques **Protein** Chemistry III (ed., R. H. Angeletti; Academic Press, N.Y.) pp. 503-515).

SUMM . . . obtaining sequence information that incorporates a data interpretation strategy based on integrating mass-to-charge ratio data obtained from a plurality of **parallel mass spectra**.

SUMM The claimed methods are applicable to any polymer, including biopolymers such as DNAs, RNAS, PNAs, **proteins**, peptides and carbohydrates, and modified forms of these polymers. The set of polymer fragments may be created by hydrolysis of. . .

DETD . . . moiety. In a currently preferred embodiment, the polymer is a biopolymer selected from, but not limited to, the following group: **proteins**, peptides, DNAs, RNAs, PNAs (peptide nucleic acids), carbohydrates and modified forms thereof.

DETD The claimed invention can be applied to the sequencing of any natural biopolymer such as **proteins**, peptides, nucleic acids, carbohydrates, etc., as well as synthetic biopolymers such as PNA and phosphotiolated nucleic acids. The ladders could. . .

DETD . . . collective truncated hydrolyzed polymer fragments. In this manner, for example, sequence information relating to the amino acid sequence of a **protein** can be obtained using carboxypeptidase Y, an agent which acts at the carboxy terminus. By using the methods disclosed herein to generate a series of **protein** hydrolysates related one to the other by consecutive, repetitive liberation of amino acid residues, the skilled artisan can reconstruct the primary sequence of the intact **protein** polymer as described in further detail below.

DETD . . . invention for this purpose. Thus the above-described subtractive-type sequencing method, through which repetitive removal of successive amino-terminal residues from a **protein** polymer can occur, can also be accomplished with hydrolyzing agents other than enzymes as disclosed herein.

DETD As disclosed herein, this strategy can be applied to the sequencing of any natural biopolymer such as **proteins**, peptides, nucleic acids, carbohydrates, etc. as well as synthetic biopolymers such as PNA and phosphothiolated nucleic acids. The ladders can. . .

CLM What is claimed is:

5. The method of claim 4 wherein the biopolymer is selected from the group consisting of DNAs, RNAs, PNAs, **proteins**, peptides, carbohydrates and modified forms thereof.

22. The method of claim 21 wherein the biopolymer is selected from the